

AN INTERPOLATION METHOD FOR OBTAINING THERMODYNAMIC PROPERTIES NEAR SATURATED LIQUID AND SATURATED VAPOR LINES

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ABSTRACT

The availability and proper utilization of fluid properties is of fundamental importance in the process of mathematical modeling of propulsion systems. Real fluid properties provide the bridge between the realm of pure analytics and empirical reality. The two most common approaches used to formulate thermodynamic properties of pure substances are fundamental (or characteristic) equations of state (Helmholtz and Gibbs functions) and a piecemeal approach that is described, for example, in Adebiyi and Russell (1992). This paper neither presents a different method to formulate thermodynamic properties of pure substances nor validates the aforementioned approaches. Rather its purpose is to present a method to be used to facilitate the accurate interpretation of fluid thermodynamic property data generated by existing property packages. There are two parts to this paper. The first part of the paper shows how efficient and usable property tables were generated, with the minimum number of data points, using an aerospace industry standard property package (based on fundamental equations of state approach). The second part describes an innovative interpolation technique that has been developed to properly obtain thermodynamic properties near the saturated liquid and saturated vapor lines.

INTRODUCTION

For many years, computer-based mathematical models have been used to analyze thermodynamic systems, and it is no doubt an effective way to save time and money for doing parametric studies and/or what-if scenarios. The quality of a model depends on many factors such as assumptions, governing equations, boundary condition definition, and of course thermodynamic properties. Having good fluid property data not only improves the model's accuracy, but it also makes the model easier to debug. For example, when the modeling results are in question relative to, say, hardware testing results, it is necessary to determine if there are any errors in the model. If the fluid property routines are not trusted, then they may be contributing factors to the errors; however, if fluid property routines have been verified, then they are no longer suspects, and the modeler can be confident that the errors are elsewhere.

The fundamental (or characteristic) equations of state and the "piecemeal" method are the two most common approaches used to formulate thermodynamic properties of pure substances. The fundamental equations of state are derived from a combination of the first and second laws of thermodynamics along with the Helmholtz and the Gibbs functions. Using these laws and functions, the complete list of thermodynamic properties can then be obtained by differentiating the fundamental equations of state. On the other hand, the thermodynamic properties equations for the "piecemeal" approach, which are developed by using the specific heat and pressure, specific volume, and temperature data for each phase of a substance, are typically the integrals of the pertinent functions.

Ideally, a simple set of equations would be integrated into a code (just like conservation of mass, momentum, and energy) and used to obtain every thermodynamic property for all phases of a given substance, but, unfortunately, that is not the case. So the next best thing is to use existing property packages, which contain complex equations with many coefficients, to get the fluid property data necessary for use within the mathematical models. However, it is very time consuming to use standard property packages within a computer simulation; therefore, property tables are used to save computational time. With that in mind, there are two parts to this paper. The first part of the paper shows how efficient and usable property tables were generated, with the minimum number of data points, using an aerospace industry standard property package (based on fundamental equations of state approach). The second part describes an innovative interpolation technique that has been developed to properly obtain thermodynamic properties near the saturated liquid and saturated vapor lines.

RESULTS AND DISCUSSION

PROPERTY PACKAGES

There are a number of property packages commercially available. NIST, MIPROPS, and GASPAK are a few examples of those packages and were used in this paper for comparison testing. As a demonstration of the techniques discussed in this paper, selected sets of data points for oxygen were chosen to represent every part of an entire fluid region. Non-saturated properties were generated using pressure (P) and temperature (T) as inputs, while saturated properties were obtained using pressure and quality (X). Table 1 compares density (ρ) and constant pressure specific heat (C_p) from the three property packages listed above, and as expected, the thermodynamic properties for those data points are very similar. Thus, for this example, it is a matter of personal preference as to which property package to use to generate property tables. The authors have decided to use GASPAK due to its relative ease of implementation.

		NIST	MIPROPS	GASPAK
P = 220 psia; X = 0 Saturated Liquid	ρ (lbm/ft ³)	57.6702	57.6710	57.6687
	C_p (Btu/lbm-°R)	0.4951	0.4950	0.4951
P = 220 psia; X = 1 Saturated Vapor	ρ (lbm/ft ³)	3.6691	3.6760	3.6688
	C_p (Btu/lbm-°R)	0.3548	0.3500	0.3548
P = 520 psia; T = 200 °R Subcooled Liquid	ρ (lbm/ft ³)	64.9515	65.0110	64.9514
	C_p (Btu/lbm-°R)	0.4238	0.4220	0.4238
P = 70 psia; T = 500 °R Superheated Vapor	ρ (lbm/ft ³)	0.4192	0.4200	0.4192
	C_p (Btu/lbm-°R)	0.2208	0.2210	0.2208
P = 5000 psia; T = 700 °R Supercritical	ρ (lbm/ft ³)	19.6892	19.7160	19.6889
	C_p (Btu/lbm-°R)	0.2755	0.2760	0.2755

Table 1. Property Data for Different Property Packages

PROPERTY TABLES

The first step in creating computationally efficient fluid property tables involves the evaluation of the property state space. Real fluid property tables were generated using the GASPAK property package (based on fundamental equations of state approach) by inputting pressures and enthalpies. The fundamental goal of this effort was to minimize the number of pressure-enthalpy values necessary to generate property tables that fully described the fluid. To accomplish this, a computer program was created which indirectly allows the user to determine how many pressure-enthalpy pairs are necessary in order to achieve a prescribed interpolation error. Thus, the desired accuracy of the results across the region of fluid properties considered is used to determine the expanse of the tables generated.

First, the program evaluates fluid properties along the saturated liquid and vapor lines to determine the necessary number of pressure points and their values so that the interpolation error along these lines would be within the specified error. This is illustrated in Figure 1 (a). Then the fluid property data is divided into two regions, sub-critical and supercritical, for further evaluation. After obtaining the pressure values for saturated lines, the program then determines pressure-enthalpy values for the supercritical region. This is a more involved process than what have been done for the saturated lines, but more or less, the methodology remains functionally similar. The program starts out with the lowest enthalpy value and determines the necessary number of pressure points for the supercritical region so that the interpolation error along that enthalpy line would be within the specified error. Similarly, the program starts out with the critical pressure (lowest pressure point for the supercritical region) and determines the necessary number of enthalpy points required to fulfill the specified interpolation error limits. The process is repeated up and across the entire supercritical region until the grid is generated as shown in Figure 1 (b). This same technique could be used for the sub-critical region, and one would find that the sub-critical enthalpies are almost identical to the supercritical enthalpies. So for the sub-critical

region, it is acceptable to use the same pressure values as the saturated lines, and likewise, the same enthalpy values as the supercritical region. The entire grid is shown in Figure 1 (c). The aforementioned program could be used to determine the grid for each fluid property at a time or to determine the grid for multiple fluid properties at the same time. In other words, one could use the program to obtain the grid for density and then use the program again to obtain the grid for specific heat, and most likely, the two grids would not be the same. On the other hand, one could use the program to determine only one grid that would satisfy the specified interpolation error limits for both density and specific heat. Figure 2 demonstrates what the grids would look like for oxygen temperature and density, and as expected, the grids get finer in the vicinity of the critical point.

INTERPOLATION METHODS

After having evaluated the state space for a given fluid property, the data is compiled into tables. Then, a means of utilizing these tables in an accurate manner across the full state space must be applied. Two tables were generated for each thermodynamics property. The first table (Property Table 1) only includes saturated vapor and saturated liquid properties, while the second table (Property Table 2) contains everything else but saturated properties. For the supercritical region and much of the space of the sub-critical region, the table-reading method used is straightforward double interpolation of Table 2. For points within the dome (or saturation envelope), data along the saturation lines (Property Table 1) are used along with fluid quality to determine composite fluid properties. However, for a small part of the sub-critical region, a special interpolation technique is required for cases where one or more data points within Property Table 2 falls inside the saturation dome. Figure 3 shows fourteen possible cases near the saturated lines where the special interpolation method is required in order to retrieve reasonable property data from the generated tables.

To see how the special interpolation technique works, let us consider saturated liquid Case 2 as defined in Figure 3 and as shown in Figure 4 within the state space. The top two data points within the interpolation rectangle (enclosed by four unshaded circular dots – from Property Table 2) lie inside the saturation envelope; therefore, they will not be used in the interpolation process. Instead, only the bottom two data points are used along with two other data points from the saturated liquid line (unshaded square dots – from Property Table 1). By using the input pressure (P) and data from Property Table 1, the saturated properties are then calculated and shown as a shaded square dot on the saturated liquid line. In the same way, the other properties (shaded circular dot) are computed by using the same input pressure and data from Property Table 2. Finally, the properties of interest are determined by interpolating between the newfound properties using the input enthalpy (H). This methodology is also used for the other thirteen cases defined in Figure 3; however, some of the other cases are not as straightforward as the example case.

Now let us look at another case, saturated vapor Case 6 as defined in Figure 3 and as shown in Figure 5 within the state space, where it is not as straightforward as the saturated liquid Case 2. Again, the interpolation rectangle is formed by four unshaded circular dots (from Property Table 2), and the bottom left data point will not be used in the interpolation process because it lies inside the saturated envelope. First, it is necessary to determine the pressure (P_{cross}) at which the saturated vapor line crosses the lower enthalpy line (H_{lo}) of the interpolation rectangle and then to see if the input pressure (P) is higher than or lower than P_{cross} . So within saturated vapor Case 6, there are two sub-cases. One case is where P is less than P_{cross} , and the other case is where P is greater than or equal to P_{cross} . This example case falls into the latter sub-case. Next by using P_{cross} and data from Property Table 1, the saturated properties are calculated and shown as a shaded square dot on the saturated vapor line. Now the property for H_{lo} (shaded triangular dot) is computed by interpolating between the newfound saturated properties and the bottom right data point from Property Table 2 using the input pressure. Similarly using the same input pressure, the property for H_{hi} (shaded circular dot) is obtained by interpolating between the top two data points from Property Table 2, and finally the properties of interest are determined by interpolating between the H_{lo} and H_{hi} properties using the input enthalpy (H).

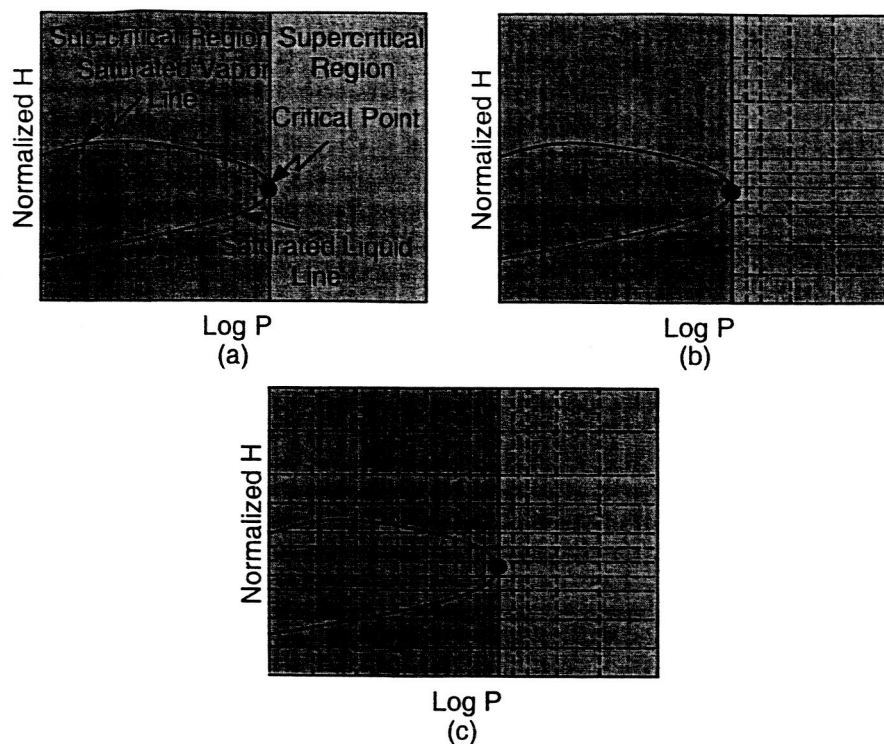


Figure 1. Pressure-Enthalpy Grid

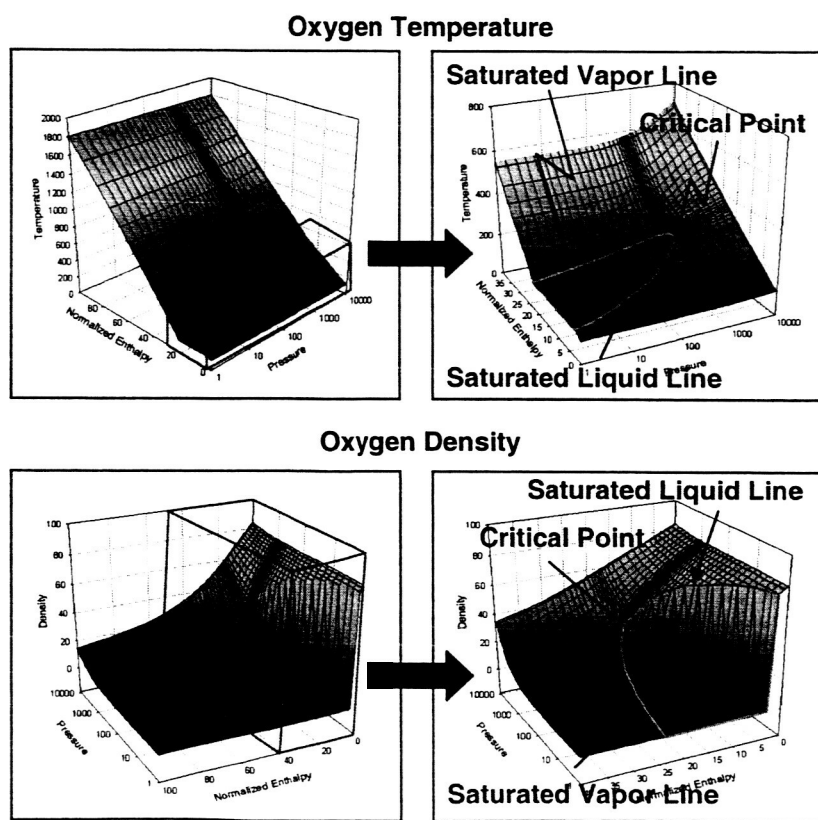


Figure 2. Property Data for Oxygen Temperature and Density

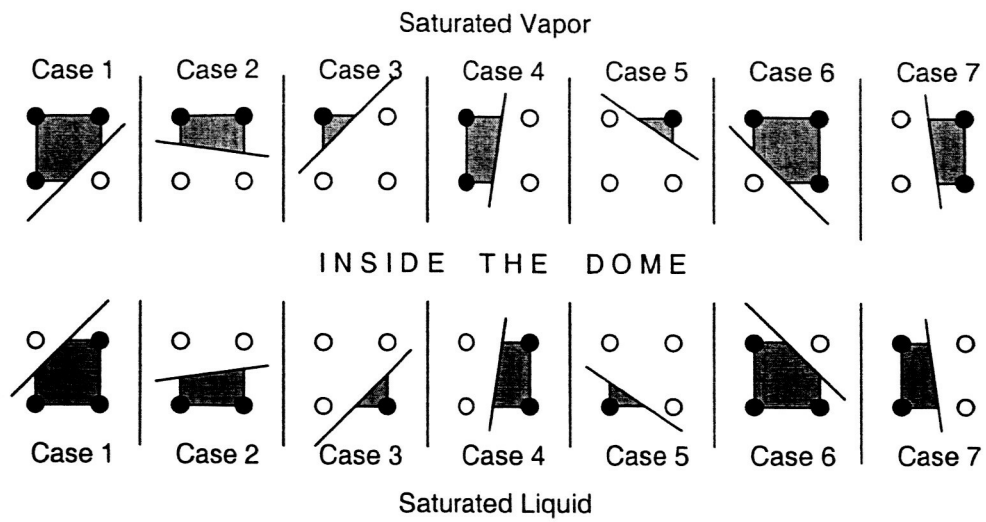


Figure 3. Possible Special Interpolation Cases Near Saturated Lines

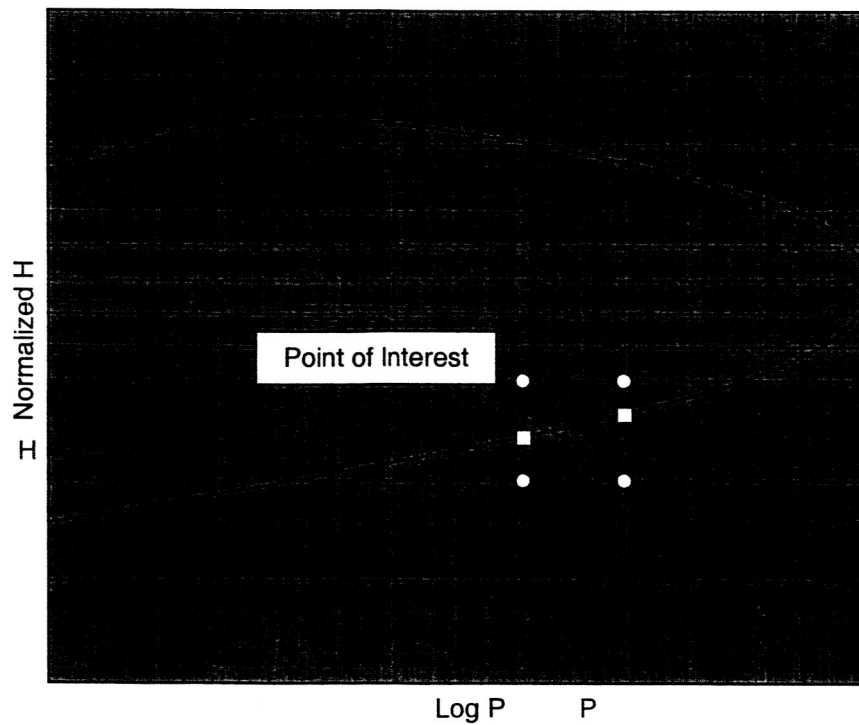


Figure 4. Saturated Liquid Case 2

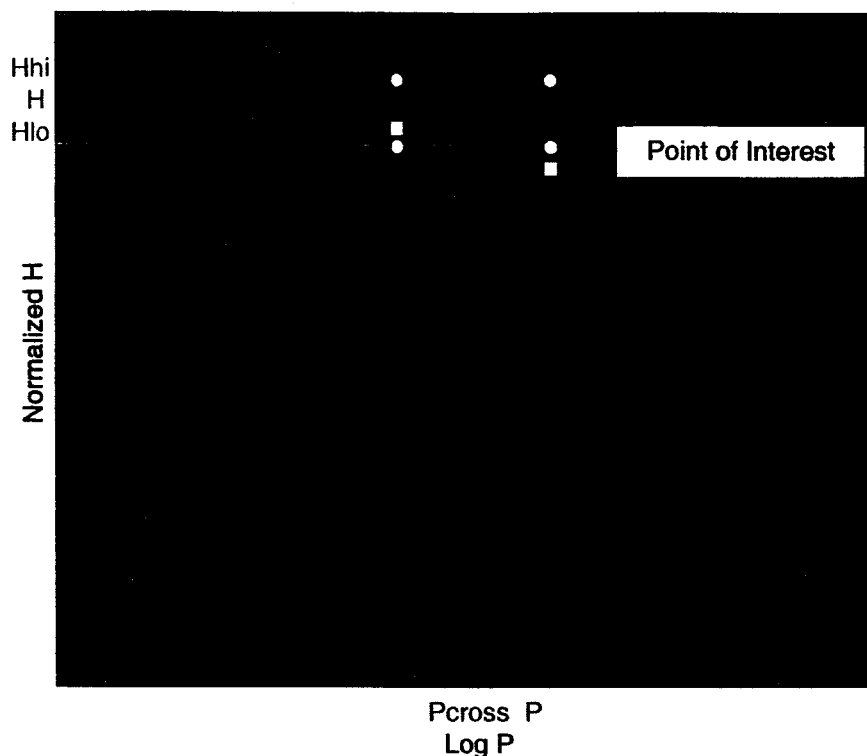


Figure 5. Saturated Vapor Case 6

PROPERTY TABLES VERSUS PROPERTY PACKAGES

As stated earlier, the main reason for using property tables instead of property packages within a computer simulation is to save computational time, but how much time is actually saved by using property tables? To answer this question, a simple model was built where there is only one control volume (node), and the thermodynamic properties for that volume were determined 50,000 times by using the same pressure and enthalpy each time. When property tables were used, it only took about 13 seconds to get the oxygen properties; however, it took almost 25 minutes (24 minutes and 54 seconds) when GASPAC was used to perform the same task. One might be surprised by how long it took when using the property package, but remember that GASPAC was called within the computer simulation. There is no doubt that it would take a lot less time if GASPAC is used outside of the computer simulation, but the basis for building property tables is not to use them outside of a computer simulation, but to use them within a computer simulation.

Now let us consider a mathematical model for a hypothetical facility used for component testing and see how long it would take for the model to run. Let us assume that the model is comprised of 25 control volumes. Fifteen of those volumes have only one fluid, either a fuel or an oxidizer, and the other ten volumes have two fluids, a fuel and an inert fluid or an oxidizer and an inert fluid. First, let us consider the one-fluid volumes. In order to get property data for a one-fluid volume, a computer code that would be used in this example needs to call a property package (or property tables) three times, so the total number of property call for fifteen one-fluid volumes is 45 times. For a two-fluid volume, the computer code needs to call a property package six times, three times per fluid. Since there are two fluids, it is assumed that the fluids would mix together and become a homogeneous mixture, and in order to get reasonable properties for the mixture, it is assumed that on average it would take about three iterations. So for a two-fluid volume, it would require a total of 18 property calls, and consequently, the total number of property call for ten two-fluid volumes is 180 times. Hence, the total number of property call for this twenty-five-volume example is 225 times. Now let us assume that it would take, on average, three iterations for the overall system model to converge for each time step, so the total number of property call

per converged time step is 675 times. Finally, if the simulation is run for five seconds with a time step of 0.001 second then the total number of property call is 3,375,000 times. As noted earlier for every 50,000 property calls, it would take about 13 seconds when using property tables and about 25 minutes when using property package. So for this example, it would take about 15 minutes versus 28 hours to finish a five seconds simulation, and that is a lot of time saving. This example is illustrated in Table 2, and it represents a fairly typical mathematical modeling situation.

		One-Fluid Volume	Two-Fluid Volume
One Time Step	Number of property call for one volume	3	6
	Homogeneous mixture – Number of iteration	1	3
	Total number of property call for one volume	3	18
	Number of volume in the model	15	10
	Number of property call for each volume type	45	180
	Total number of property call for the model	225	
Number of iteration for each time step to converge		3	
Total number of property call for each time step		675	
Number of time step (5 seconds simulation, 0.001 second time step)		5000	
Total number of property call for the simulation		3,375,000	
		Property Tables	Property Package (GASPAK)
Time required for every 50,000 property calls		13 sec.	24 min. and 54 sec.
Total simulation time		~15 min.	~28 hrs.

Table 2. Twenty-Five-Volume Model

SUMMARY AND CONCLUSIONS

There are two parts to this paper. The first part of the paper shows how efficient and usable property tables were generated, with the minimum number of data points, using the GASPAK property package. The numbers of data points in the tables were indirectly determined from the specified acceptable error between interpolated values from the tables and values obtained from the property package. The second part of the paper describes how thermodynamics properties were retrieved from the tables. For the most part, the interpolation method used is straightforward use of property tables. However, for the fourteen cases near the saturation lines, the special interpolation method is required in order to obtain reasonable property data from the generated tables. As a result, a new interpolation routine was developed to handle both sub-critical and supercritical regions.

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